Dynamic Data-Driven Event Reconstruction for Atmospheric Releases

(A collaborative effort between Computation, Energy & Environment, NAI and Engineering)

Project Overview
The role of an event reconstruction capability in a case of an atmospheric release is to characterize the source by answering the critical questions – *How much material was released? When? Where?* and *What are the potential consequences?* Accurate estimation of the source term is essential to accurately predict plume dispersion, effectively manage the emergency response, and mitigate consequences in a case of an atmospheric release of hazardous material. We are developing a capability that seamlessly integrates observational data streams with predictive models in order to provide probabilistic estimates of unknown source term parameters consistent with both data and model predictions. Our approach utilizes Bayesian inference with stochastic sampling using Markov Chain and Sequential Monte Carlo methodology. The inverse dispersion problem is reformulated into a solution based on efficient sampling of an ensemble of predictive simulations, guided by statistical comparisons with data.

Project Goals
We are developing a flexible and adaptable data-driven event-reconstruction capability for atmospheric releases that provides (1) quantitative probabilistic estimates of the principal source-term parameters (e.g., the time-varying release rate and location); (2) predictions of increasing fidelity as an event progresses and additional data become available; and (3) analysis tools for sensor network design and uncertainty studies. Our computational framework incorporates multiple stochastic algorithms, operates with a range and variety of atmospheric models, and runs on multiple computer platforms, from workstations to large-scale computing resources. Our final goal is a multi-resolution capability for both real-time operational response and high fidelity multi-scale applications.

Relevance to LLNL Mission
This project directly contributes to the Laboratory's homeland and national security mission by addressing a critical need for atmospheric release event reconstruction tools to support the rapidly growing number of operational detection, warning, and incident characterization systems being developed and deployed by the Department of Homeland Security (e.g., BioWatch, BWIC system, national BioSurveillance Initiative) and Department of Energy (e.g., Nuclear Incident Response Team assets and deployments). The event reconstruction and sensor siting tools developed by this LDRD are targeted for integration into the next-generation National Atmospheric Release Advisory Center and DHS's new Inter-agency Modeling and Atmospheric Analysis Center, based at LLNL.

FY05 Accomplishments and Results
In FY05, we: (1) demonstrated efficiency and robustness of MCMC capability with the NARAC 3D Lagrangian particle dispersion model LODI using concentration

measurements from a ~10 km -scale tracer field experiment; (2) developed a hybrid MCMC-SMC methodology and demonstrated its effectiveness in characterizing releases from complex, multiple sources; (3) used optimization methods to develop a prototype sensor network design tool; (4) implemented a computational fluid dynamics model for the simulation of urban dispersion into the MCMC capability and tested it using data from the Oklahoma City - Joint Urban 2003 experiment; (5) developed a computational framework including MCMC, SMC, and hybrid algorithms on massively parallel platforms; (6) explored methods for incorporating alternative input data types (e.g., remote sensing, qualitative, imagery); and (7) significantly enhanced performance on massively parallel platforms for efficient event reconstruction of complex atmospheric releases.

Proposed work for FY06
In FY06 we will: (1) extend the event reconstruction capability to handle complex continental scale atmospheric releases; (2) implement data, input parameter, and internal model error quantification procedures into the computational framework; (3) implement a multi-resolution capability for more efficient source characterization; (4) continue developing and testing efficient stochastic sampling and convergence algorithms; (5) demonstrate methods for incorporating alternative input data types (e.g., remote sensing, qualitative, imagery); and (6) continue performance enhancement of the computational framework on the range of platforms for efficient event reconstruction of complex atmospheric releases.

(a)   (b)   (c)
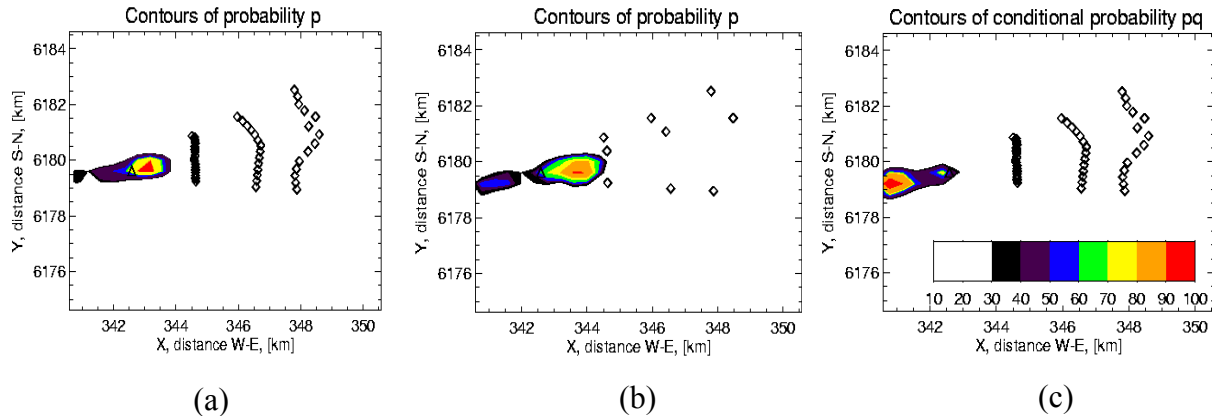
An example of event reconstruction using an operational three-dimensional Lagrangian particle dispersion model and data from the Copenhagen field tracer experiment. In all of the panels, color contours represent the probability distribution of the source location; the actual source is denoted with a triangle, while the sensors are denoted with diamonds. In panel (a) event reconstruction using data from all 51 sensors is presented; in panel (b) source characterization based on data from only nine sensors is presented – notice that the confidence interval is larger than in case (a), indicating higher uncertainty; in panel (c) results obtained using all 51 sensors out of which 30% of the sensors were broken in some way (i.e., giving false positives, false negatives, or stuck on a wrong concentration) are shown – the effect of inaccurate data is evident through the bias in the solution; however the robustness of the methodology is demonstrated.
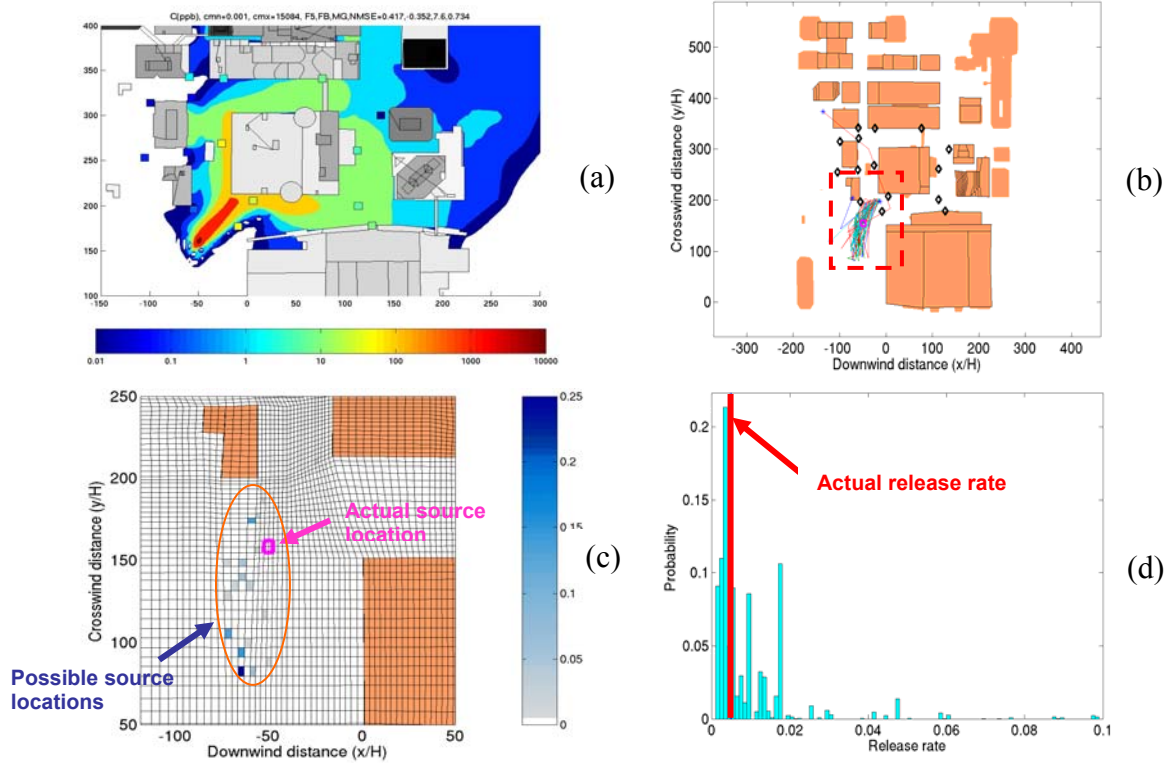
An example of event reconstruction for a release in an urban environment using a three-dimensional computational fluid dynamics code and concentration measurements from the field tracer experiment Joint Urban 2003 in Oklahoma City. In panel (b) four Markov Chains exploring source location are presented; panel (c) presents a magnification of a red dashed-line rectangle from panel (b) with probability distribution of source location presented as colored squares, where gray color represent low value of probability density and dark blue color represents high value of probability density; the pink rectangle denotes the actual source location; in panel (d) the probability distribution (histogram) of the source release rate is presented; the red line denotes actual release rate.

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